Aminotrimethylene phosphonic acid
6419-19-8 | DTXSID2027624

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.80 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.56e-01

Confidence level: 5.48e-01

Nearest Neighbors from the Training Set

Image not found
Aminotrimethylene phosphonic
acid
Measured: 3.34
Predicted: 2.80

Image not found
Glyphosine
Measured: 9.43e-01
Predicted: 9.05e-01

Image not found
Etidronic acid
Measured: 3.35
Predicted: 3.04

Image not found
Phosphonic acid, [1,6-
hexanediylbis[nitrilobis(methylene)]]tetrakis-
Measured: 3.05e-02
Predicted: 4.19e-02